

National Aeronautics and Space Administration



Quantum Computing at NASA: Current Status

Dr. Rupak Biswas

*Director, Exploration Technology Directorate
Manager, NASA High End Computing Capability (HECC) Project*

NASA Ames Research Center, Moffett Field, Calif., USA

6th International Conference on Space Mission Challenges for Information Technology (SMC-IT)

www.nasa.gov

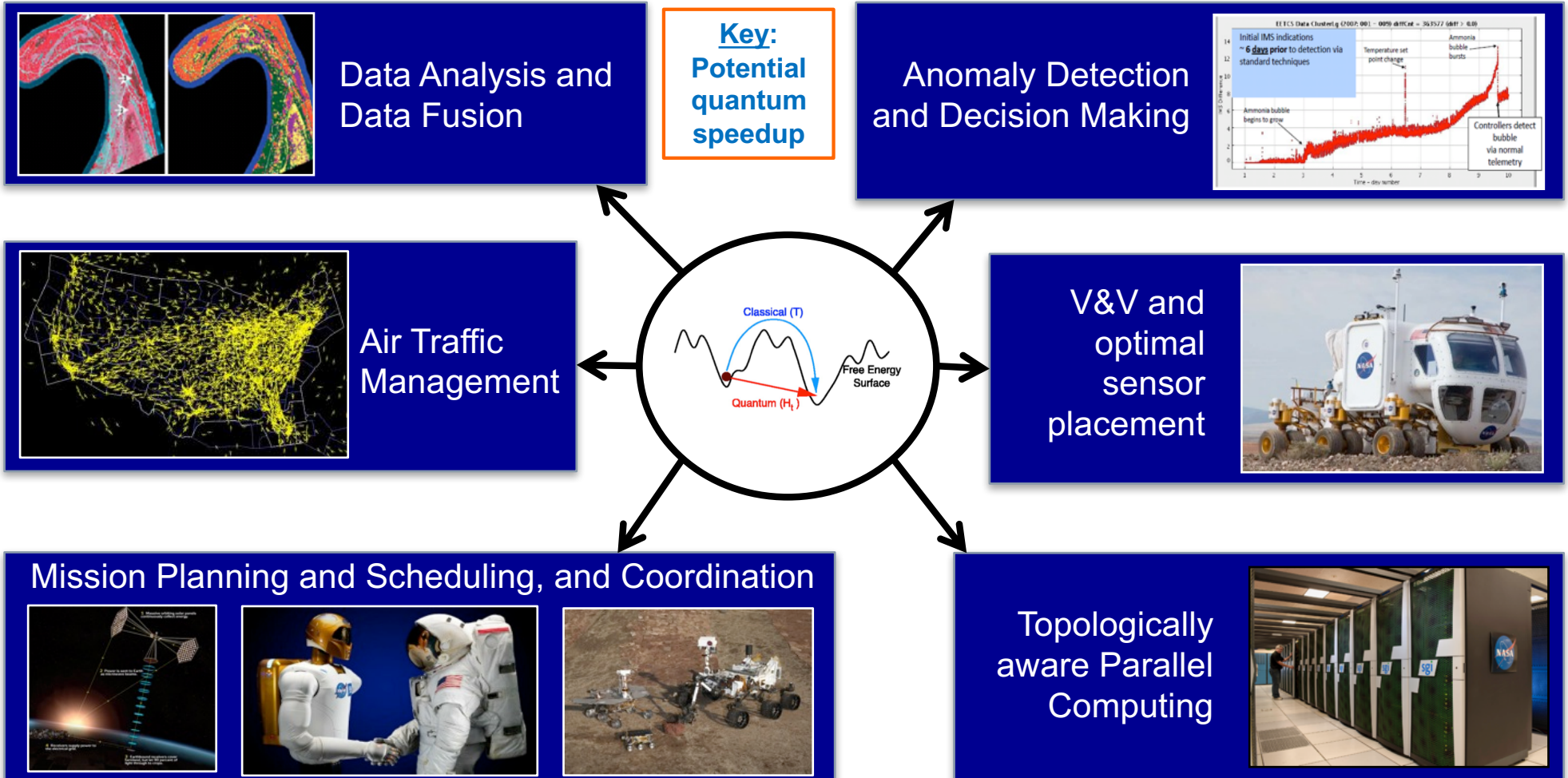
Alcala de Henares, Spain, 28 September 2017



National Aeronautics and
Space Administration



Why Quantum Computing at NASA



Common Feature: Intractable (NP-hard / NP-complete) problems!



National Aeronautics and
Space Administration

Ames

Discovery • Innovations • Solutions

QuAIL: Quantum Artificial Intelligence Laboratory

Brief Development Timeline

2000–2011: Occasional NASA research on quantum computing, including seminal papers on adiabatic quantum computing & quantum annealing

Jan 2012: NASA organizes the First Quantum Future Technologies

Conference attracting eminent researchers worldwide and participation from companies such as Google and D-Wave Systems

Nov 2012: NASA signs innovative 3-way Non-Reimbursable Space Act Agreement (NRSAA) with Google and USRA

Jan 2013: Site preparations begin at NASA Ames using Center investment funds for installation of D-Wave quantum annealer

Sept 2013: 512-qubit D-Wave 2 system comes on-line at Ames

June 2014: AFRL funding for research in quantum annealing

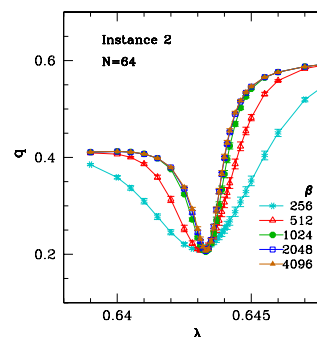
Aug 2014: IARPA funding for MIT-LL led QEO collaboration among NASA, TAMU, ETH-Z, UC Berkeley, and MIT

July 2015: Upgraded D-Wave 2X quantum annealer comes on-line with over 1000 qubits

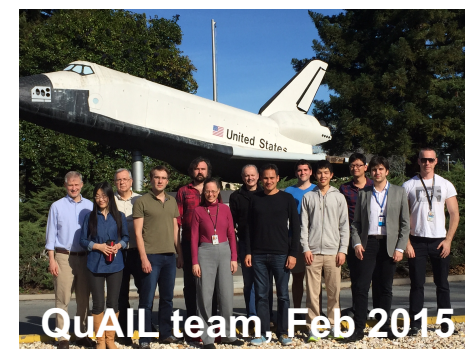
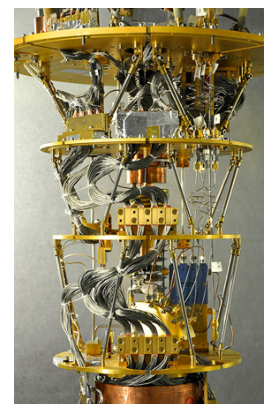
Feb 2017: NASA signs NRSAA with Rigetti Computing for collaborative work on their prototype universal quantum processor

April 2017: Latest upgrade underway for D-Wave system with over 2000 qubits

May 2017: NASA to lead T&E effort for IARPA QEO program



Phys. Rev. Lett. 104, 020502 (2010)



QuAIL team, Feb 2015

QuAIL team has published 40+ papers since 2012



Office of the Director of National Intelligence
IARPA
BE THE FUTURE



QUANTUM
ENHANCED
OPTIMIZATION





National Aeronautics and
Space Administration



NASA QuAIL Team Focus

Long Term

- Determine the breadth and range of quantum computing applications
- Explore potential quantum algorithms and applications of relevance to NASA
- Evaluate, influence, and utilize emerging quantum hardware
 - Develop programming principles, compilation strategies, etc.
 - Characterize the hardware capabilities, noise, etc.
 - Evaluate and implement the most promising NASA applications
- Projections based on fundamental understanding of quantum physics

Ongoing Efforts

- Initial target: Quantum Annealing
 - Only significant quantum hardware available are quantum annealers from D-Wave Systems
 - Currently the most prominent quantum heuristic
 - Widely applicable to optimization problems, and sampling for ML
 - Early hardware used to develop intuitions and identify potential
- Near-term target: Emerging quantum computing hardware
 - Small universal quantum systems
 - Advanced quantum annealers
 - Alternative approaches to optimization, sampling for ML, etc.

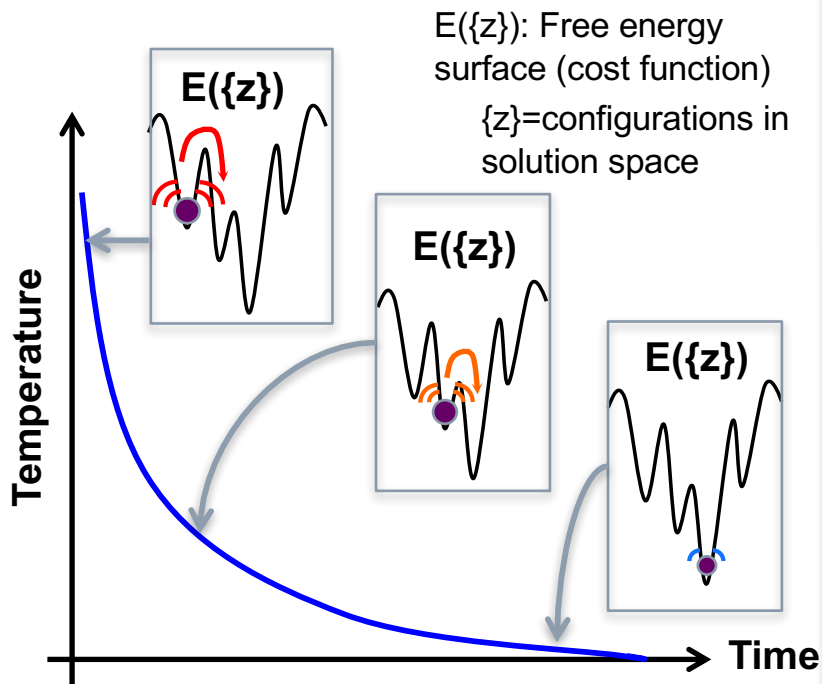


Foundational Theory of Quantum Annealing

Simulated Annealing

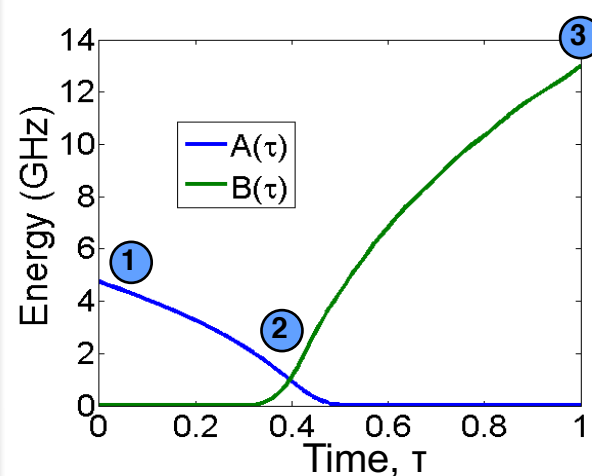
(Kirkpatrick et al., 1983)

- **Algorithm:** Start with high temperature; then, gradually reduce intensity of thermal fluctuations to obtain optimal configuration
- Transitions between states via jumping over barriers due to thermal fluctuations



Quantum Annealing

(Finnila et al., 1994, Kadawaki & Nishimori, 1998, Farhi et.al., 2001)



- **Algorithm:** Start with large amplitude $A(\tau)$ responsible for quantum fluctuations; then, gradually turn it off while turning on the cost function of interest $B(\tau)$
- Transitions between states via tunneling through barriers due to quantum fluctuations

①
 $E(\{z\}, \tau=0)$

Initialize in an easy to prepare full quantum superposition

②
 $E(\{z\}, \tau < 1)$

Quantum states explored by quantum tunneling

③
 $E(\{z\}, \tau=1)$

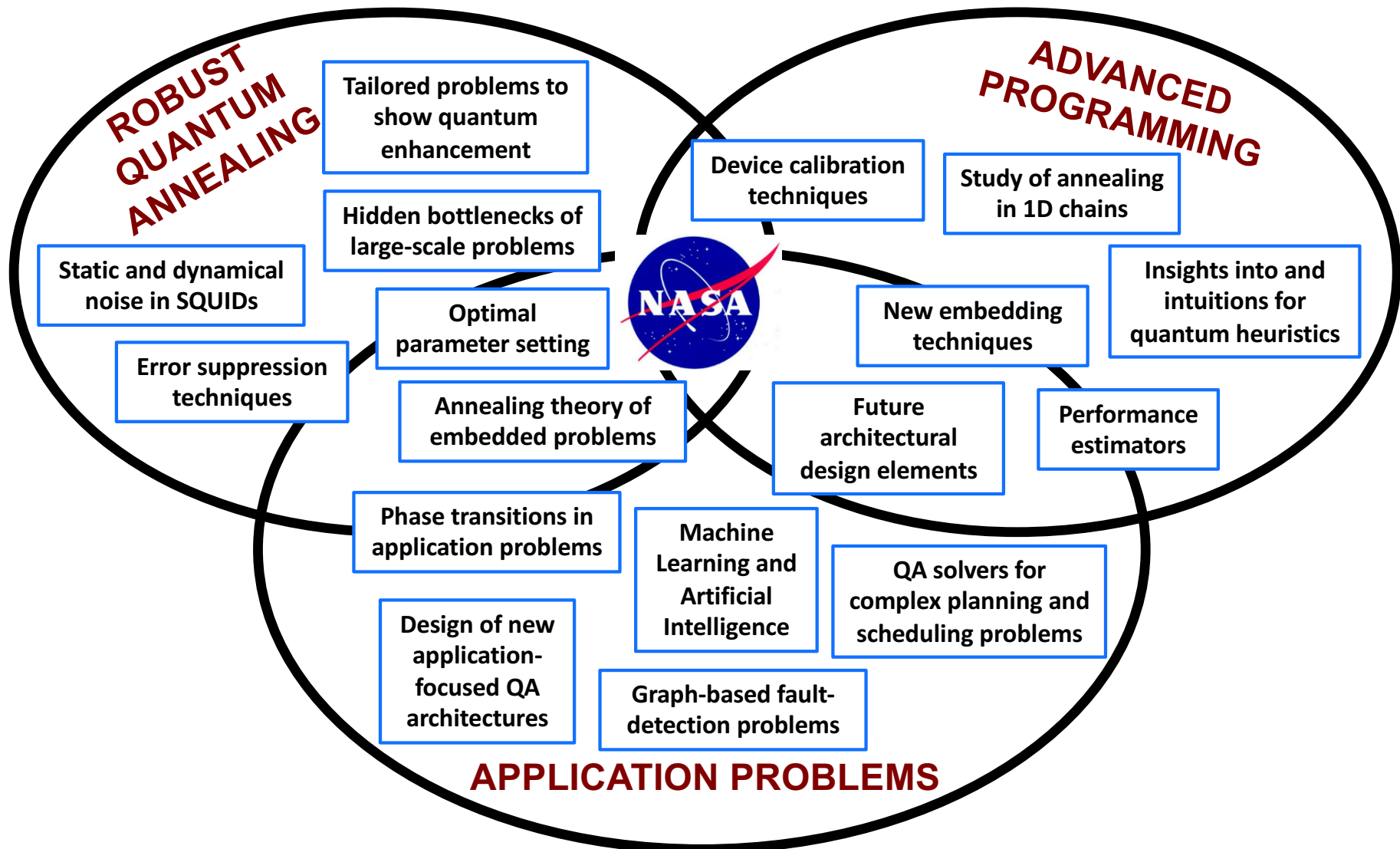
Final state a bit string encoding the solution with probability



National Aeronautics and
Space Administration



NASA Quantum Research Approach



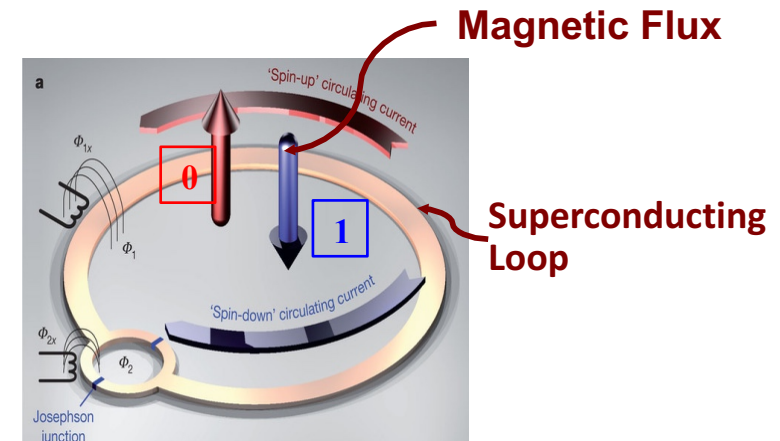
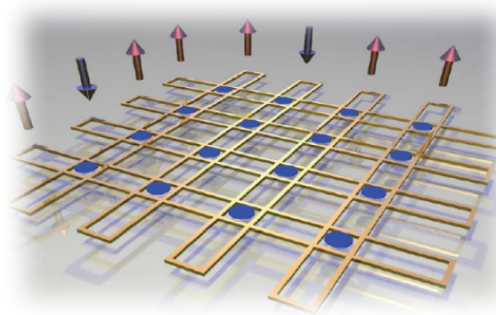
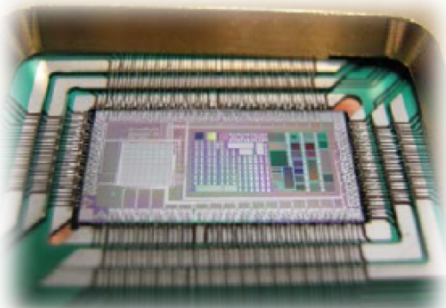
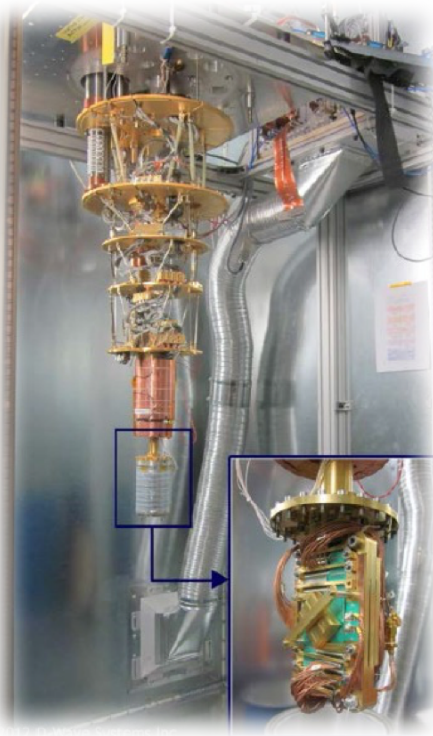


National Aeronautics and
Space Administration



D-Wave System Hardware

- Collaboration with Google and USRA led to installation of system at NASA Ames in 2013
- Started with 512-qubit Vesuvius processor (currently upgrading to 2000-qubit Whistler)
- 10 kg metal in vacuum at ~ 15 mK
- Magnetic shielding to 1 nanoTesla
- Protected from transient vibrations
- Single annealing takes $20 \mu\text{s}$
- Typical run of 10,000 anneals (incl. reset & readout takes ~ 4 sec)
- Uses 12 kW of electrical power



Focused on solving discrete optimization problems using quantum annealing 7



National Aeronautics and
Space Administration



D-Wave System Capability

The system solves only one binary optimization problem:

Given $\{ h_j, J_{ij} \}$, find $\{ s_k = \pm 1 \}$
that minimizes

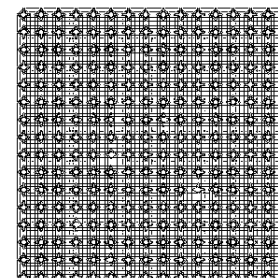
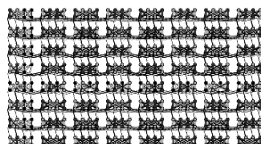
$$\xi(s_1, \dots, s_N) = \sum_{j=1}^N h_j s_j + \sum_{i,j \in E} J_{ij} s_i s_j$$



National Aeronautics and
Space Administration



Vesuvius to Washington to Whistler



D-Wave Two	D-Wave 2X	D-Wave 2000Q
512 (8x8x8) qubit “Vesuvius” processor	1152 (8x12x12) qubit “Washington” processor	2048 (8x16x16) qubit “Whistler” processor
509 qubits working – 95% yield	1097 qubits working – 95% yield	2038 qubits working – 97% yield
1472 <i>J</i> programmable couplers	3360 <i>J</i> programmable couplers	6016 <i>J</i> programmable couplers
20 mK max operating temperature (18 mK nominal)	15 mK max operating temperature (13 mK nominal)	15 mK max operating temperature (<i>nominal to be measured</i>)
5% and 3.5% precision level for <i>h</i> and <i>J</i>	3.5% and 2% precision level for <i>h</i> and <i>J</i>	<i>To be measured</i>
20 us annealing time 12 ms programming time	5 us annealing time (4X better) 12 ms programming time	5 us annealing time 9 ms programming time (25% better) New: anneal offset, pause, quench
6 graph connectivity per qubit	6 graph connectivity per qubit	6 graph connectivity per qubit



Programming the D-Wave System

1 Map the target combinatorial optimization problem into QUBO

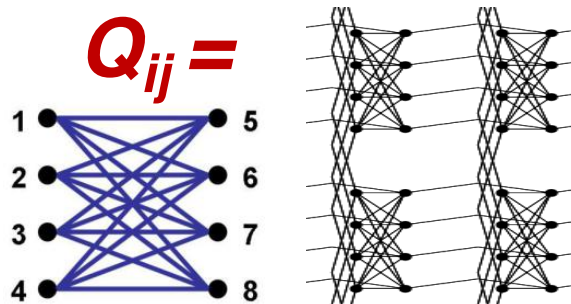
No general algorithms but smart mathematical tricks (penalty functions, locality reduction, etc.)

$$\alpha_{ijk} z_i z_j z_k$$
$$\alpha_{ijk} y_{ij} z_k + \beta_{ijk} (3y_{ij} - 2z_i y_{ij} - 2z_j y_{ij} + z_i z_j)$$
$$\sum_{ij} Q_{ij} z_i z_j \rightarrow \sum_i h_i s_i + \sum_{i,j} J_{ij} s_i s_j$$

Mapping not needed for random spin-glass models

2 Embed the QUBO coupling matrix in the hardware graph of interacting qubits

D-Wave qubit hardware connectivity is a Chimera graph, so embedding methods mostly based on heuristics

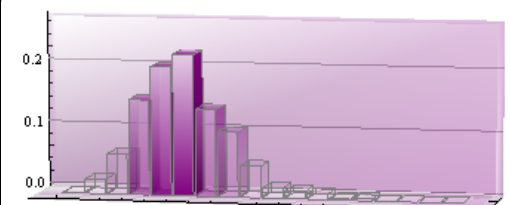


Embedding not needed for native Chimera problems

3 Run the problem several times and collect statistics

Use symmetries, permutations, and error correction to eliminate the systemic hardware errors and check the solutions

Probability



Solution's energy/cost

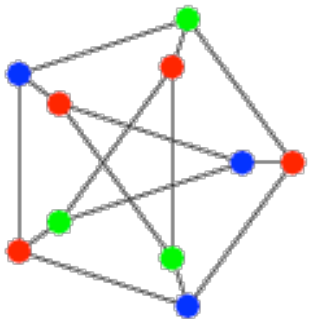
Performance can be improved dramatically with smart pre-/post-processing



Mapping to QUBO: Graph Coloring Example

Graph Coloring Problem:

Assign one of k colors to each vertex so that no two vertices sharing an edge have the same color



Costing cases



(1) No color or Multi-colored



(2) Same color for connected vertices

Binary variable:

$$x_{v,c} = \begin{cases} 1 & \text{vertex } v \text{ with color } c \\ 0 & \text{vertex } v \text{ not with color } c \end{cases}$$

Violation of requirements encoded as cost:

- (1) unique assignment: Each vertex v must be assigned exactly one color:

$$H_v^{(unique)} = \left(\sum_{c \in C} x_{v,c} - 1 \right)^2 \Leftrightarrow \sum_{c \in C} x_{v,c} = 1$$

- (2) Connected vertices cannot use the same color

$$H_{v,v',c}^{(exclude)} = x_{v,c} x_{v',c} \text{ if } vv' \in E$$

Final QUBO form:

$$H = \sum_v H_v^{(unique)} + \sum_{v,v' \in E} \sum_c H_{v,v',c}^{(exclude)}$$

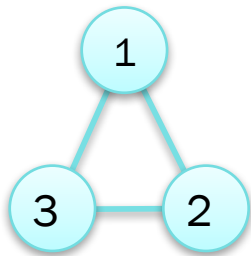
H = 0 corresponds to a valid coloring



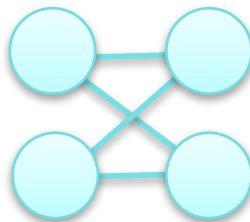
Embedding the QUBO

Embed a triangle onto a bipartite graph

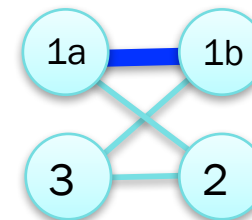
original QUBO



hardware connectivity



QUBO embedded



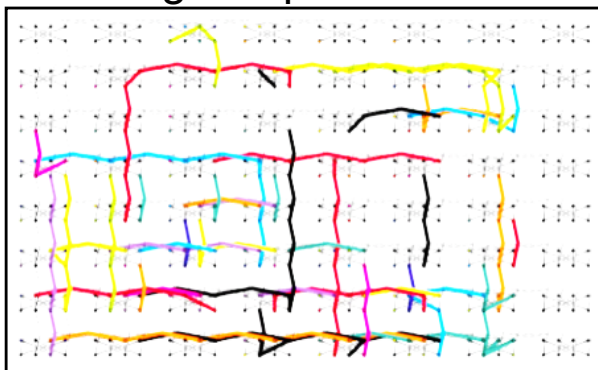
$$H_0 = J_{12}x_1x_2 + J_{23}x_2x_3 + J_{13}x_1x_3$$

$$H_1 = J_{12}x_{1a}x_2 + J_{23}x_2x_3 + J_{13}x_{1b}x_3 + \underline{J_{\text{Ferro}}}x_{1a}x_{1b}$$

Strong, but not too strong, ferromagnetic coupling between physical qubits x_{1a} and x_{1b} encourages them to take the same value, thus acting as a single logical qubit x_1

Embedding a realistic problem instance:

Physical qubits on each colored path represent one logical qubit



H_0 and H_1 have the same ground state but the energy landscape of the search space differs

Current research investigation: How best to set the magnitude of these “strong” couplings to maximize probability of success

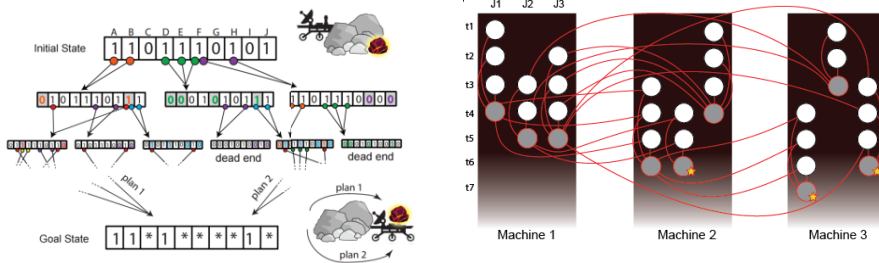


National Aeronautics and
Space Administration

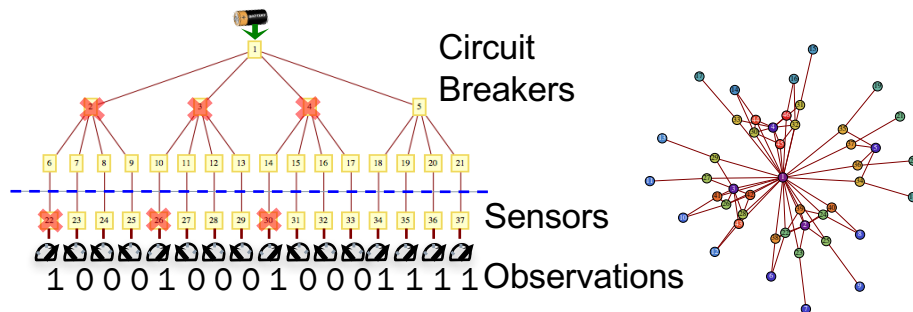
Ames
Discovery • Innovations • Solutions

Current NASA Research in Applications

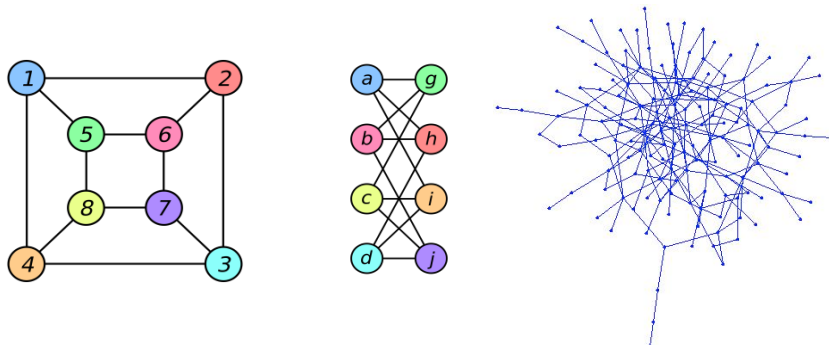
Complex Planning and Scheduling



Graph-based Fault Detection



Graph Isomorphism

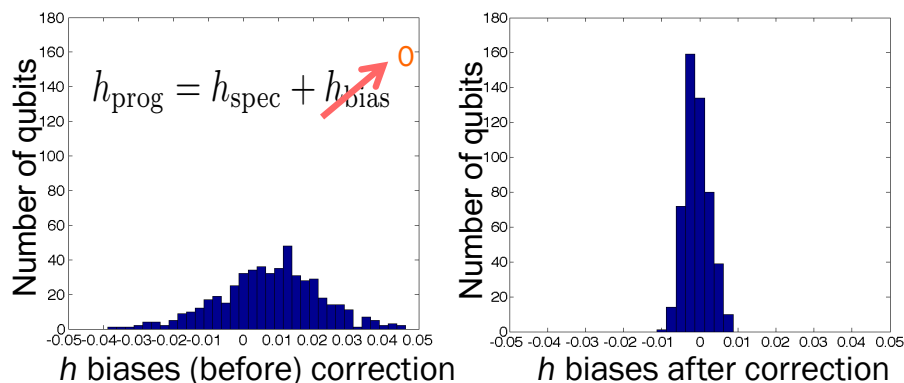


- General **Planning Problems** (e.g., navigation, scheduling, asset allocation) can be solved on a quantum annealer
- Developed a quantum solver for **Job Shop Scheduling** that pre-characterizes instance ensembles to design optimal embedding and run strategy – tested at small scale (6x6) but potentially could solve intractable problems (15x15) with 10x more qubits
- Analyzed simple graphs of **Electrical Power Networks** to find the most probable cause of multiple faults – easy and scalable QUBO mapping, but good parameter setting (e.g., gauge selection) key to finding optimal solution – now exploring digital circuit **Fault Diagnostics and V&V**
- **Subgraph Matching Problems** are common in applications of interest to the intelligence community – similarly, finding **Longest Matching Sequences** important in genomics and bioinformatics

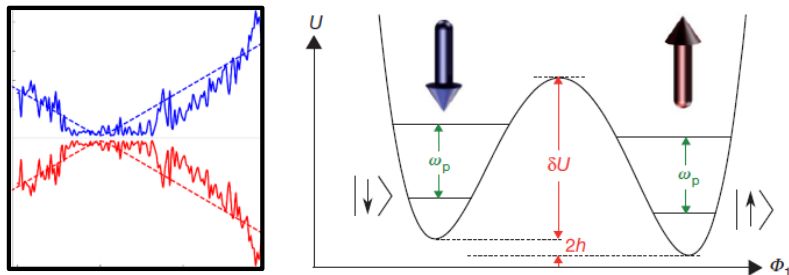


Current NASA Research in Quantum Physics

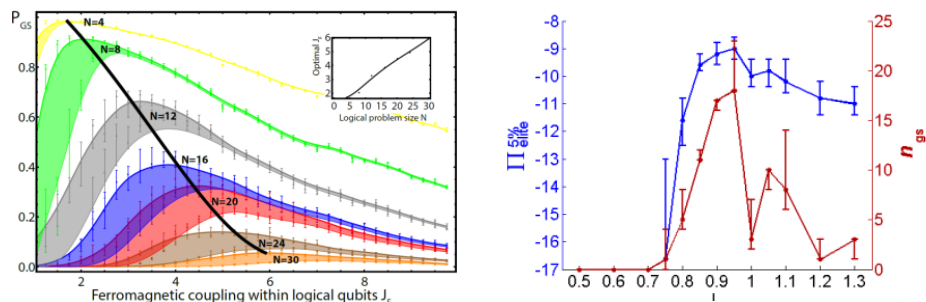
Calibration of Quantum Annealers



Effect of Noise on Quantum Annealing



Optimal Embedding & Parameter Setting



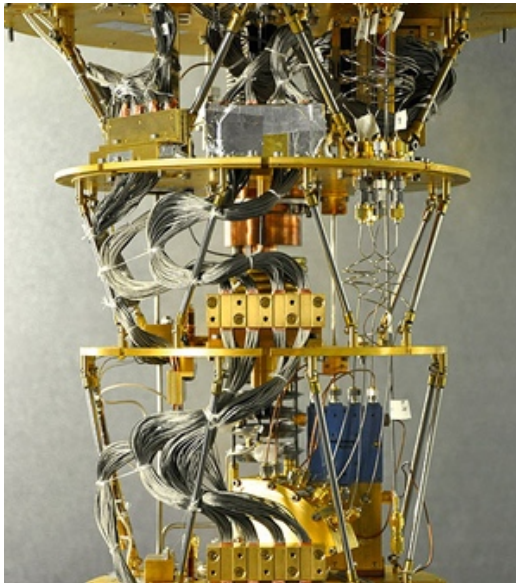
- Developed technique to determine and correct **residual persistent biases** in the programmable parameters of quantum annealers (h and J) – correction significantly improves performance and reliability (reduction in variability)
- First **realistic noise analyses** show how low-frequency noise dramatically affects the performance of quantum annealers – results being used to design hardware improvements
- Limited hardware connectivity makes embedding challenging – good runtime parameters determined by considering the **nature and dynamics of chains** – quick scans can be used to predict performance of extensive scans
- Small instances of **hard problems at phase transitions** in combinatorial optimization are intractable – they can be designed by looking at solvability phase transitions
- Predict **tractability of application problems** by studying the scaling of energy gaps and density of bottlenecks in spin glass phase



National Aeronautics and
Space Administration

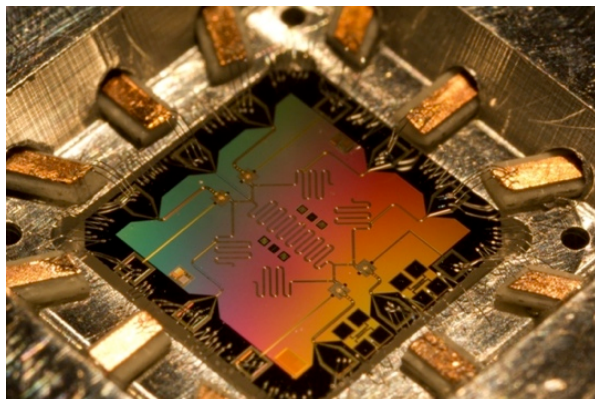


Emerging Quantum Hardware

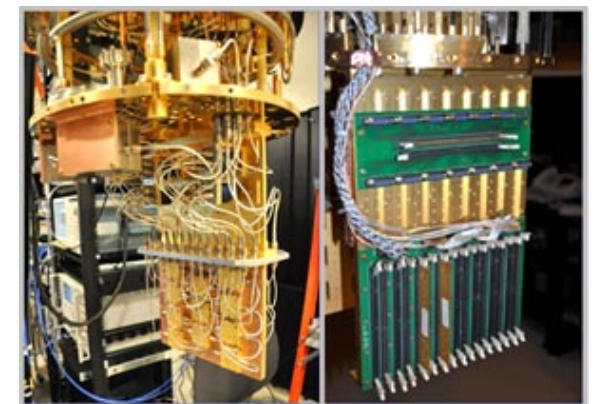


D-Wave Systems

- What should we do with the emerging and exciting, but limited, quantum computational devices?
 - Still too small to be useful for solving practical problems
- Couple of possibilities:
 - Quantum supremacy
 - ***Develop intuitions for quantum heuristics***



Google Martinis Lab



MIT-LL



Quantum Heuristics

Conjecture: Quantum Heuristics will significantly broaden applications of quantum computing

Known quantum algorithms for a few dozen problems with a provable quantum advantage

Everything Else! (incl. most practical problems)

- Even for classical computations
 - Provable bounds hard to obtain
 - Robust analysis is just too difficult
- Best classical algorithm not known for most problems
- Ongoing development of classical heuristic approaches
 - Analyzed empirically: run and see
- Emerging quantum hardware enables evaluation of heuristic quantum algorithms

Handful of proven limitations on quantum computing



Designing and Vetting Quantum Heuristics

1. Generate suggestions for good quantum heuristics, e.g.,
 - Hypotheses for computational utilization of quantum effects
 - Algorithmic structures that encompass quantum algorithms with provable benefits
 - Compelling arguments for advantage in larger-scale application problems; robustness
2. Design experiments running tailored problems on available hardware to confirm or deny hypotheses
3. Analyze and compare with classical algorithms, incl. those inspired by these quantum intuitions

Pool of quantum properties

Quantum interference

Quantum entanglement

Quantum tunneling

Quantum sampling

Quantum measurement

Non-commutative quantum operators

Quantum discord

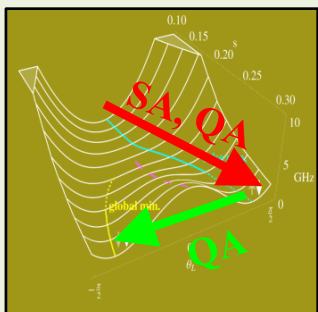
Quantum adiabatic theorem

Quantum contextuality



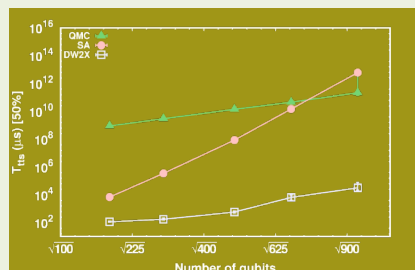
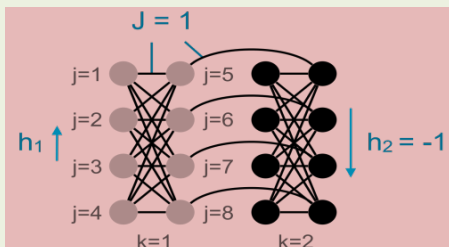
Case Study: Quantum Tunneling & Annealing

1. Intuition for quantum annealing



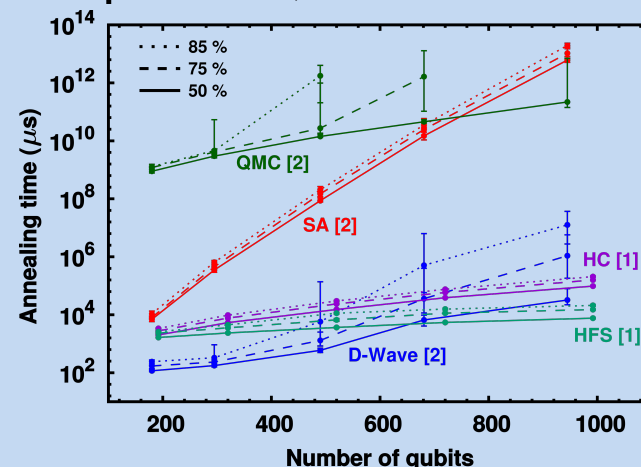
- K. Kechedzhi, V. Smelyanskiy, *Open System Quantum Annealing in Mean Field Models with Exponential Degeneracy*, PRX (2016)
- S. Knysh, *Computational Bottlenecks of Quantum Annealing*, arXiv:1506.08608
- D. Venturelli, S. Mandrà, S. Knysh, B. O'Gorman, R. Biswas, V. Smelyanskiy, *Quantum Optimization of Fully-Connected Spin Glasses*, PRX (2015)
- H. Nishimori, J. Tsuda, S. Knysh, *Comparative Study of the Performance of Quantum Annealing and Simulated Annealing*, PRE (2014)
- V. Smelyanskiy, D. Venturelli, A. Perdomo-Ortiz, S. Knysh, M. Dykman, *Quantum Annealing via Environment-Mediated Quantum Diffusion*, arXiv:1511.02581

2. Tailored problems for quantum tunneling



- V. Denchev, S. Boixo, S. Isakov, N. Ding, R. Babbush, V. Smelyanskiy, J. Martinis, H. Neven, *What is the Computational Value of Finite Range Tunneling?*, PRX (2016)
- S. Boixo, V. Smelyanskiy, A. Shabani, S. Isakov, M. Dykman, V. Denchev, M. Amin, A. Smirnov, M. Mohseni, H. Neven, *Computational Multi-qubit Tunneling in Programmable Quantum Annealers*, Nat. Comm. (2016)

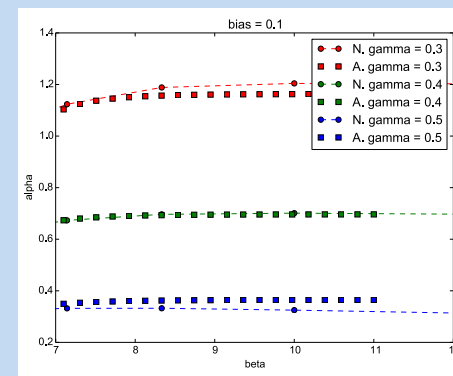
3a. Comparison, incl. new techniques



- S. Mandrà, Z. Zhu, W. Wang, A. Perdomo-Ortiz, H. Katzgraber, *Strengths and Weaknesses of Weak-Strong Cluster Problems: A Detailed Overview of State-of-the-Art Classical Heuristics vs. Quantum Approaches*, PRA (2016)

3b. And analysis

Instanton method:
exponential scaling
of escape rate in
QMC equals
tunneling rate in QA



- Z. Jiang, V. Smelyanskiy, S. Isakov, S. Boixo, G. Mazzola, M. Troyer, H. Neven, *Scaling Analysis and Instantons for Thermally-Assisted Tunneling and Quantum Monte Carlo Simulations*, arXiv:1603.01293 (2016)



National Aeronautics and
Space Administration

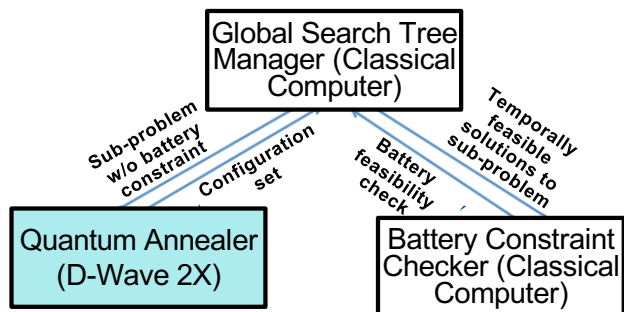
Ames
Discovery • Innovations • Solutions

Quantum-Classical Hybrid Approaches

Exploits complementary properties of quantum and classical solvers:

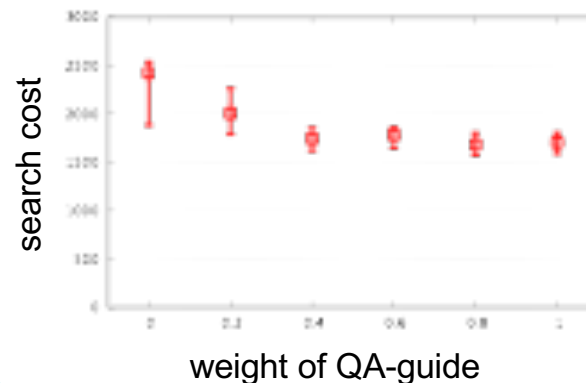
- Quantum annealing provides heuristic
- Classical processing ensures complete search
- Enlarges application domain of quantum annealers

QA-guided tree search

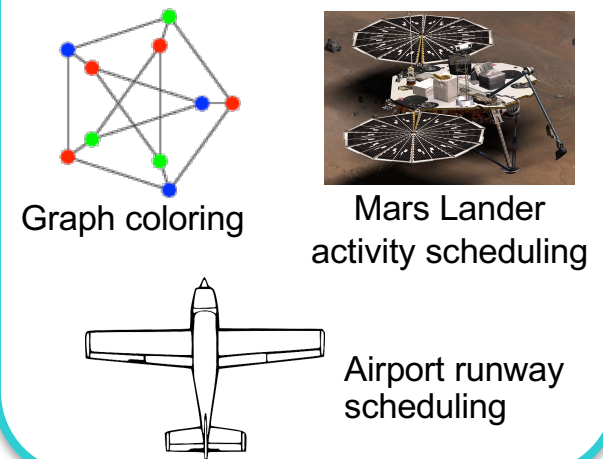


Quantum annealer samples the search space of a relaxed version of the original problem

QA results exploited to guide the tree search



Application domains tested



On-going study of hybrid methods

Incorporating more advanced quantum-classical interaction using techniques such as Logic Benders Decomposition, column generation, and large neighborhood search

- T. Tran, M. Do, E. Rieffel, J. Frank, Z. Wang, B. O'Gorman, D. Venturelli, J. Beck, **A Hybrid Quantum-Classical Approach to Solving Scheduling Problems**, SOCS'16
- T. Tran, Z. Wang, M. Do, E. Rieffel, J. Frank, B. O'Gorman, D. Venturelli, J. Beck, **Explorations of Quantum-Classical Approaches to Scheduling a Mars Lander Activity Problem**, Workshops AAAI'16



Universities Space Research Association (USRA)

Academia and Industry Engagement Program

A program to enable a diversity of research in quantum computing, and develop the next-generation workforce with expertise in quantum computing

<http://www.usra.edu/quantum/rfp/>

Free Compute Time

Available for qualified research projects from universities and industry. Projects selected through a competitive process

Workshops, Seminars, Training

University and industry researchers invited to participate in workshops and other educational opportunities

Visiting Scientist Program

Universities and industry can sponsor a visiting scientist to work at NASA Ames with QuAIL team members

Joint Proposals

University and industry scientists invited to collaborate on proposals to sponsored research programs



National Aeronautics and
Space Administration

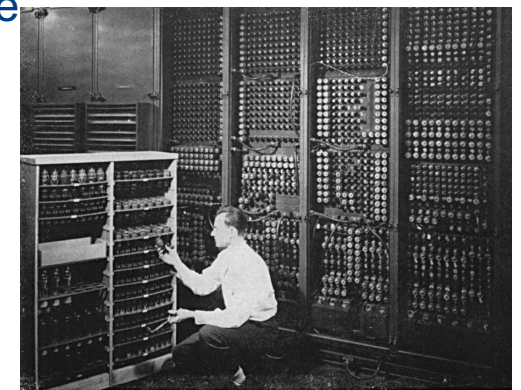


Conclusions

- Understanding and harnessing the fundamental power of quantum computing is a formidable challenge that requires:
 - New insights in physics and mathematics
 - Innovations in computer and computational science
 - Breakthroughs in engineering design to produce robust, reliable, scalable technologies
- NASA QuAIL team has successfully demonstrated that discrete optimization problems can be run on quantum annealers
 - Effectively using such systems needs judicious mapping, embedding, execution strategies
- Exciting decade in quantum computing ahead of us
 - Compilation and performance capabilities of today's annealers are improving rapidly
 - New and better quantum algorithms, particularly quantum heuristics, are emerging
 - Small-scale universal quantum computers are becoming available

ENIAC (1946), the first “general-purpose” computer

The task of taking a problem and mapping it onto the machine was complex, and usually took weeks. After the program was figured out on paper, the process of getting the program "into" ENIAC by manipulating its switches and cables took additional days. This was followed by a period of verification and debugging [...] (source: <http://en.wikipedia.org/wiki/ENIAC>)



Replacing a bad tube meant checking among ENIAC's 19,000 possibilities.